Automated Docking Screens: A Feasibility Study

Journal of Medicinal Chemistry 52, 5712-5720 DOI: 10.1021/jm9006966

Citation Report

#	Article	IF	CITATIONS
1	Molecular Docking Screens Using Comparative Models of Proteins. Journal of Chemical Information and Modeling, 2009, 49, 2512-2527.	5.4	132
2	The Drug Discovery Portal: A Computational Platform for Identifying Drug Leads from Academia. Current Pharmaceutical Design, 2010, 16, 1697-1702.	1.9	3
3	Structureâ€Based Approaches to Target Fishing and Ligand Profiling. Molecular Informatics, 2010, 29, 176-187.	2.5	132
4	A Structure-Based Approach for Mapping Adverse Drug Reactions to the Perturbation of Underlying Biological Pathways. PLoS ONE, 2010, 5, e12063.	2.5	47
5	e-LEA3D: a computational-aided drug design web server. Nucleic Acids Research, 2010, 38, W615-W621.	14.5	107
6	Opal web services for biomedical applications. Nucleic Acids Research, 2010, 38, W724-W731.	14.5	42
7	Docking Validation Resources: Protein Family and Ligand Flexibility Experiments. Journal of Chemical Information and Modeling, 2010, 50, 1986-2000.	5.4	153
8	Advances and Challenges in Protein-Ligand Docking. International Journal of Molecular Sciences, 2010, 11, 3016-3034.	4.1	418
9	History of 3D pharmacophore searching: commercial, academic and open-source tools. Drug Discovery Today: Technologies, 2010, 7, e255-e262.	4.0	7
10	Rapid Context-Dependent Ligand Desolvation in Molecular Docking. Journal of Chemical Information and Modeling, 2010, 50, 1561-1573.	5.4	276
11	Recent advances and method development for drug target identification. Trends in Pharmacological Sciences, 2010, 31, 82-88.	8.7	102
12	Targeting SDF-1/CXCL12 with a Ligand That Prevents Activation of CXCR4 through Structure-Based Drug Design. Journal of the American Chemical Society, 2010, 132, 7242-7243.	13.7	68
13	Virtual Screening of Selective Multitarget Kinase Inhibitors by Combinatorial Support Vector Machines. Molecular Pharmaceutics, 2010, 7, 1545-1560.	4.6	55
14	Tackling the challenges posed by target flexibility in drug design. Expert Opinion on Drug Discovery, 2010, 5, 347-359.	5.0	38
15	Structure-based discovery of prescription drugs that interact with the norepinephrine transporter, NET. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 15810-15815.	7.1	120
16	SwissDock, a protein-small molecule docking web service based on EADock DSS. Nucleic Acids Research, 2011, 39, W270-W277.	14.5	1,396
17	<i>AADS</i> - An Automated Active Site Identification, Docking, and Scoring Protocol for Protein Targets Based on Physicochemical Descriptors. Journal of Chemical Information and Modeling, 2011, 51, 2515-2527.	5.4	113
18	Reactome: a database of reactions, pathways and biological processes. Nucleic Acids Research, 2011, 39, D691-D697.	14.5	1,391

#	Article	lF	CITATIONS
19	Construction and Test of Ligand Decoy Sets Using MDock: Community Structure–Activity Resource Benchmarks for Binding Mode Prediction. Journal of Chemical Information and Modeling, 2011, 51, 2107-2114.	5.4	21
20	Ligand discovery from a dopamine D3 receptor homology model and crystal structure. Nature Chemical Biology, 2011, 7, 769-778.	8.0	285
21	The unusual extended C-terminal helix of the peroxisomal α/β-hydrolase Lpx1 is involved in dimer contacts but dispensable for dimerization. Journal of Structural Biology, 2011, 175, 362-371.	2.8	19
22	Identification of Alternative Binding Sites for Inhibitors of HIV-1 Ribonuclease H Through Comparative Analysis of Virtual Enrichment Studies. Journal of Chemical Information and Modeling, 2011, 51, 1986-1998.	5.4	35
23	Statistical Potential for Modeling and Ranking of Protein–Ligand Interactions. Journal of Chemical Information and Modeling, 2011, 51, 3078-3092.	5.4	69
24	Protection Against Neuroinflammation by Promoting Co-activation of G Protein– Growth Factor Signaling and Metabolic Flexibility in the Brain. , 2011, , 325-346.		0
25	Prediction of Ligand Binding Using an Approach Designed to Accommodate Diversity in Protein-Ligand Interactions. PLoS ONE, 2011, 6, e23215.	2.5	5
26	Current Trends in Virtual High Throughput Screening Using Ligand-Based and Structure-Based Methods. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 872-888.	1.1	33
27	Virtual Decoy Sets for Molecular Docking Benchmarks. Journal of Chemical Information and Modeling, 2011, 51, 196-202.	5.4	55
28	iScreen: world's first cloud-computing web server for virtual screening and de novo drug design based on TCM database@Taiwan. Journal of Computer-Aided Molecular Design, 2011, 25, 525-531.	2.9	127
29	VSDMIP 1.5: an automated structure- and ligand-based virtual screening platform with a PyMOL graphical user interface. Journal of Computer-Aided Molecular Design, 2011, 25, 813-824.	2.9	18
30	Challenges and advances in computational docking: 2009 in review. Journal of Molecular Recognition, 2011, 24, 149-164.	2.1	273
31	EfficientIn SilicoAssay of Inhibitors of Hepatitis C Virus RNA-Dependent RNA Polymerase by Structure-Based Virtual Screening andIn VitroEvaluation. Assay and Drug Development Technologies, 2011, 9, 290-298.	1.2	8
32	Rosetta FlexPepDock web server—high resolution modeling of peptide–protein interactions. Nucleic Acids Research, 2011, 39, W249-W253.	14.5	351
33	Pocketome: an encyclopedia of small-molecule binding sites in 4D. Nucleic Acids Research, 2012, 40, D535-D540.	14.5	149
34	Freely Accessible Databases of Commercial Compounds For High- Throughput Virtual Screenings. Current Topics in Medicinal Chemistry, 2012, 12, 866-877.	2.1	50
35	iFad: an integrative factor analysis model for drug-pathway association inferenceâ€. Bioinformatics, 2012, 28, 1911-1918.	4.1	27
36	Microwave-assisted synthesis, molecular docking and antitubercular activity of 1,2,3,4-tetrahydropyrimidine-5-carbonitrile derivatives. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 7539-7542.	2.2	26

#	Article	IF	CITATIONS
37	How to Benchmark Methods for Structure-Based Virtual Screening of Large Compound Libraries. Methods in Molecular Biology, 2012, 819, 187-195.	0.9	5
38	Structure–Activity Relationships and Molecular Modeling of 1,2,4-Triazoles as Adenosine Receptor Antagonists. ACS Medicinal Chemistry Letters, 2012, 3, 715-720.	2.8	17
39	Structure-based drug screening for G-protein-coupled receptors. Trends in Pharmacological Sciences, 2012, 33, 268-272.	8.7	258
40	High Selectivity of the γ-Aminobutyric Acid Transporter 2 (GAT-2, SLC6A13) Revealed by Structure-based Approach. Journal of Biological Chemistry, 2012, 287, 37745-37756.	3.4	49
41	Directory of Useful Decoys, Enhanced (DUD-E): Better Ligands and Decoys for Better Benchmarking. Journal of Medicinal Chemistry, 2012, 55, 6582-6594.	6.4	1,574
42	Sanjeevini: a freely accessible web-server for target directed lead molecule discovery. BMC Bioinformatics, 2012, 13, S7.	2.6	169
43	Life Beyond Kinases: Structure-Based Discovery of Sorafenib as Nanomolar Antagonist of 5-HT Receptors. Journal of Medicinal Chemistry, 2012, 55, 5749-5759.	6.4	68
44	Chemical informatics uncovers a new role for moexipril as a novel inhibitor of cAMP phosphodiesterase-4 (PDE4). Biochemical Pharmacology, 2013, 85, 1297-1305.	4.4	17
45	Functional Validation of Virtual Screening for Novel Agents with General Anesthetic Action at Ligand-Gated Ion Channels. Molecular Pharmacology, 2013, 84, 670-678.	2.3	19
46	Complementarity between in Silico and Biophysical Screening Approaches in Fragment-Based Lead Discovery against the A2A Adenosine Receptor. Journal of Chemical Information and Modeling, 2013, 53, 2701-2714.	5.4	65
47	Molecular modelling and simulations in cancer research. Biochimica Et Biophysica Acta: Reviews on Cancer, 2013, 1836, 1-14.	7.4	39
48	From Heptahelical Bundle to Hits from the Haystack. Methods in Enzymology, 2013, 522, 279-336.	1.0	47
49	Functional Annotation and Three-Dimensional Structure of an Incorrectly Annotated Dihydroorotase from cog3964 in the Amidohydrolase Superfamily. Biochemistry, 2013, 52, 228-238.	2.5	8
50	Parallel strategies for an inverse docking method. , 2013, , .		1
51	A Molecular-Modeling Toolbox Aimed at Bridging the Gap between Medicinal Chemistry and Computational Sciences. International Journal of Molecular Sciences, 2013, 14, 684-700.	4.1	12
52	Muscarinic Receptors as Model Targets and Antitargets for Structure-Based Ligand Discovery. Molecular Pharmacology, 2013, 84, 528-540.	2.3	56
53	Crystal structure of the ωâ€aminotransferase from <i>Paracoccus denitrificans</i> and its phylogenetic relationship with other class III amino―transferases that have biotechnological potential. Proteins: Structure, Function and Bioinformatics, 2013, 81, 774-787.	2.6	39
54	Structure-based Discovery of Antagonists of Nuclear Receptor LRH-1. Journal of Biological Chemistry, 2013, 288, 19830-19844.	3.4	89

#	Article	IF	CITATIONS
55	Genome-Scale Screening of Drug-Target Associations Relevant to Ki Using a Chemogenomics Approach. PLoS ONE, 2013, 8, e57680.	2.5	30
56	Roles for Ordered and Bulk Solvent in Ligand Recognition and Docking in Two Related Cavities. PLoS ONE, 2013, 8, e69153.	2.5	23
57	Ligand Pose and Orientational Sampling in Molecular Docking. PLoS ONE, 2013, 8, e75992.	2.5	139
58	istar: A Web Platform for Large-Scale Protein-Ligand Docking. PLoS ONE, 2014, 9, e85678.	2.5	89
59	Comparative Modeling of Drug Target Proteinsâ~†. , 2014, , .		5
60	Software and Online Resources: Perspectives and Potential Applications. , 2014, , 233-248.		3
61	Foodinformatics., 2014,,.		15
62	Use of Freely Available and Open Source Tools for In Silico Screening in Chemical Biology. Journal of Chemical Education, 2014, 91, 602-604.	2.3	13
63	Therapeutic Applications of Ribozymes and Riboswitches. Methods in Molecular Biology, 2014, , .	0.9	0
64	Computational Approaches and Resources in Single Amino Acid Substitutions Analysis Toward Clinical Research. Advances in Protein Chemistry and Structural Biology, 2014, 94, 365-423.	2.3	22
65	A development of chimeric VEGFR2 TK inhibitor based on two ligand conformers from PDB: 1Y6A complex – Medicinal chemistry consequences of a TKs analysis. European Journal of Medicinal Chemistry, 2014, 72, 146-159.	5.5	36
66	Molecular modeling, simulation and virtual screening of ribosomal phosphoprotein P1 from Plasmodium falciparum. Journal of Theoretical Biology, 2014, 343, 113-119.	1.7	4
67	AlzPlatform: An Alzheimer's Disease Domain-Specific Chemogenomics Knowledgebase for Polypharmacology and Target Identification Research. Journal of Chemical Information and Modeling, 2014, 54, 1050-1060.	5.4	177
68	PeptiSite: A structural database of peptide binding sites in 4D. Biochemical and Biophysical Research Communications, 2014, 445, 717-723.	2.1	13
69	Challenges and advances in structure-based virtual screening. Future Medicinal Chemistry, 2014, 6, 5-7.	2.3	16
70	Identification of a Novel Inhibitor of Dengue Virus Protease through Use of a Virtual Screening Drug Discovery Web Portal. Journal of Chemical Information and Modeling, 2014, 54, 2816-2825.	5.4	52
71	More than just a GPCR ligand: structure-based discovery of thioridazine derivatives as Pim-1 kinase inhibitors. MedChemComm, 2014, 5, 507-511.	3.4	9
72	Incorporating replacement free energy of binding-site waters in molecular docking. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1765-1776.	2.6	22

#	Article	IF	CITATIONS
73	Leveraging structure for enzyme function prediction: methods, opportunities, and challenges. Trends in Biochemical Sciences, 2014, 39, 363-371.	7.5	31
74	Strategies for Improved Modeling of GPCR-Drug Complexes: Blind Predictions of Serotonin Receptors Bound to Ergotamine. Journal of Chemical Information and Modeling, 2014, 54, 2004-2021.	5.4	21
75	Structure-Based Discovery of Selective Serotonin 5-HT 1B Receptor Ligands. Structure, 2014, 22, 1140-1151.	3.3	57
76	Increasing Chemical Space Coverage by Combining Empirical and Computational Fragment Screens. ACS Chemical Biology, 2014, 9, 1528-1535.	3.4	58
77	Computational target fishing: what should chemogenomics researchers expect for the future of <i>in silico</i> drug design and discovery?. Future Medicinal Chemistry, 2014, 6, 247-249.	2.3	43
78	Inhibitors of the Cdc34 acidic loop: A computational investigation integrating molecular dynamics, virtual screening and docking approaches. FEBS Open Bio, 2014, 4, 473-484.	2.3	9
79	Repositioning of Thiourea-Containing Drugs as Tyrosinase Inhibitors. International Journal of Molecular Sciences, 2015, 16, 28534-28548.	4.1	28
80	Crystal structure of the human OX2 orexin receptor bound to the insomnia drug suvorexant. Nature, 2015, 519, 247-250.	27.8	180
81	Identification of Angiotensin Converting Enzyme Inhibitor: An In Silico Perspective. International Journal of Peptide Research and Therapeutics, 2015, 21, 107-115.	1.9	18
82	Pharmacophore modeling improves virtual screening for novel peroxisome proliferator-activated receptor-gamma ligands. Journal of Computer-Aided Molecular Design, 2015, 29, 421-439.	2.9	9
83	Automated computational screening of the thiol reactivity of substituted alkenes. Journal of Computer-Aided Molecular Design, 2015, 29, 725-735.	2.9	19
84	MTiOpenScreen: a web server for structure-based virtual screening. Nucleic Acids Research, 2015, 43, W448-W454.	14.5	159
85	Theory and Applications of Covalent Docking in Drug Discovery: Merits and Pitfalls. Molecules, 2015, 20, 1984-2000.	3.8	112
86	Molecular modeling, simulation and virtual screening of MurD ligase protein from Salmonella typhimurium LT2. Journal of Pharmacological and Toxicological Methods, 2015, 73, 34-41.	0.7	12
87	Analogues of ethionamide, a drug used for multidrug-resistant tuberculosis, exhibit potent inhibition of tyrosinase. European Journal of Medicinal Chemistry, 2015, 106, 157-166.	5.5	32
88	ZINC 15 – Ligand Discovery for Everyone. Journal of Chemical Information and Modeling, 2015, 55, 2324-2337.	5.4	2,194
89	Ynamide Click chemistry in development of triazole VEGFR2 TK modulators. European Journal of Medicinal Chemistry, 2015, 103, 105-122.	5.5	9
90	NRGsuite: a PyMOL plugin to perform docking simulations in real time using FlexAID. Bioinformatics, 2015, 31, 3856-3858.	4.1	66

#	Article	IF	CITATIONS
91	Discovery of trace amine-associated receptor 1 ligands by molecular docking screening against a homology model. MedChemComm, 2015, 6, 2216-2223.	3.4	19
92	Beware of docking!. Trends in Pharmacological Sciences, 2015, 36, 78-95.	8.7	460
93	Inverse docking method for new proteins targets identification: A parallel approach. Parallel Computing, 2015, 42, 48-59.	2.1	9
94	In silico comparative genomics analysis of Plasmodium falciparum for the identification of putative essential genes and therapeutic candidates. Journal of Microbiological Methods, 2015, 109, 1-8.	1.6	17
95	A Molecular Docking and Dynamics Study to Screen Potent Anti-Staphylococcal Compounds Against Ceftaroline Resistant MRSA. Journal of Cellular Biochemistry, 2016, 117, 542-548.	2.6	13
96	Medicinal Chemistry Strategies to Disrupt the p53–MDM2/MDMX Interaction. Medicinal Research Reviews, 2016, 36, 789-844.	10.5	71
97	Structure-Based Identification of Novel Ligands Targeting Multiple Sites within a Chemokine–G-Protein-Coupled-Receptor Interface. Journal of Medicinal Chemistry, 2016, 59, 4342-4351.	6.4	29
98	Pharmit: interactive exploration of chemical space. Nucleic Acids Research, 2016, 44, W442-W448.	14.5	219
99	Protein-protein interaction and molecular dynamics analysis for identification of novel inhibitors in Burkholderia cepacia GG4. Computational Biology and Chemistry, 2016, 65, 80-90.	2.3	7
100	An <i>in silico</i> algorithm for identifying stabilizing pockets in proteins: test case, the Y220C mutant of the p53 tumor suppressor protein. Protein Engineering, Design and Selection, 2016, 29, 377-390.	2.1	13
101	Structure-based discovery of opioid analgesics with reduced side effects. Nature, 2016, 537, 185-190.	27.8	744
102	Docking optimization, variance and promiscuity for large-scale drug-like chemical space using high performance computing architectures. Drug Discovery Today, 2016, 21, 1672-1680.	6.4	9
103	A bitter pill for type 2 diabetes? The activation of bitter taste receptor TAS2R38 can stimulate GLP-1 release from enteroendocrine L-cells. Biochemical and Biophysical Research Communications, 2016, 475, 295-300.	2.1	38
104	Introduction to Cheminformatics. Current Protocols in Bioinformatics, 2016, 53, 14.1.1-14.1.21.	25.8	15
105	Ensemble-Based Virtual Screening Led to the Discovery of New Classes of Potent Tyrosinase Inhibitors. Journal of Chemical Information and Modeling, 2016, 56, 354-367.	5.4	26
106	Computer-Aided Drug Discovery Approaches against the Tropical Infectious Diseases Malaria, Tuberculosis, Trypanosomiasis, and Leishmaniasis. ACS Infectious Diseases, 2016, 2, 8-31.	3.8	48
107	Docking and Linking of Fragments To Discover Jumonji Histone Demethylase Inhibitors. Journal of Medicinal Chemistry, 2016, 59, 1580-1598.	6.4	43
108	Identification of Phosphoribosyl-AMP cyclohydrolase, as drug target and its inhibitors in Brucella melitensis bv. 1 16M using metabolic pathway analysis. Journal of Biomolecular Structure and Dynamics, 2017, 35, 287-299.	3.5	4

#	Article	IF	CITATIONS
109	Designing and optimization of novel human LMTK3 inhibitors against breast cancer – a computational approach. Journal of Receptor and Signal Transduction Research, 2017, 37, 51-59.	2.5	12
110	Rational screening of peroxisome proliferator-activated receptor-Î ³ agonists from natural products: potential therapeutics for heart failure. Pharmaceutical Biology, 2017, 55, 503-509.	2.9	13
111	Oligopeptidase B and B2: comparative modelling and virtual screening as searching tools for new antileishmanial compounds. Parasitology, 2017, 144, 536-545.	1.5	11
112	A Molecular Docking and Dynamics Approach to Screen Potent Inhibitors Against Fosfomycin Resistant Enzyme in Clinical Klebsiella pneumoniae. Journal of Cellular Biochemistry, 2017, 118, 4088-4094.	2.6	29
113	Antithrombotic properties of JJ1, a potent and novel thrombin inhibitor. Scientific Reports, 2017, 7, 14862.	3.3	8
114	The potential role of <i>in silico</i> approaches to identify novel bioactive molecules from natural resources. Future Medicinal Chemistry, 2017, 9, 1665-1686.	2.3	27
115	Fragment-Based Discovery and Optimization of Enzyme Inhibitors by Docking of Commercial Chemical Space. Journal of Medicinal Chemistry, 2017, 60, 8160-8169.	6.4	32
116	Multi-template homology based structure prediction and molecular docking studies of protein â€~L' of Zaire ebolavirus (EBOV). Informatics in Medicine Unlocked, 2017, 9, 68-75.	3.4	10
117	Relative Binding Free Energy Calculations in Drug Discovery: Recent Advances and Practical Considerations. Journal of Chemical Information and Modeling, 2017, 57, 2911-2937.	5.4	458
118	QSAR modeling and in silico design of small-molecule inhibitors targeting the interaction between E3 ligase VHL and HIF-1 \$\$alpha \$\$ I±. Molecular Diversity, 2017, 21, 719-739.	3.9	1
119	AMMOS2: a web server for protein–ligand–water complexes refinement via molecular mechanics. Nucleic Acids Research, 2017, 45, W350-W355.	14.5	24
120	Novel CLK1 inhibitors based on N-aryloxazol-2-amine skeleton - A possible way to dual VEGFR2 TK/CLK ligands. European Journal of Medicinal Chemistry, 2017, 126, 754-761.	5.5	21
121	Chemical Informatics. , 2017, , 295-314.		0
122	Identification of small-molecule ligands that bind to MiR-21 as potential therapeutics for endometriosis by screening ZINC database and in-vitro assays. Gene, 2018, 662, 46-53.	2.2	16
123	Computational Systems Biology of Metabolism in Infection. Experientia Supplementum (2012), 2018, 109, 235-282.	0.9	6
124	Structure-based discovery of selective positive allosteric modulators of antagonists for the M ₂ muscarinic acetylcholine receptor. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E2419-E2428.	7.1	57
125	Comprehensive assessment of flexible-ligand docking algorithms: current effectiveness and challenges. Briefings in Bioinformatics, 2018, 19, 982-994.	6.5	37
126	Molecular modeling studies to explore the binding affinity of virtually screened inhibitor toward different aminoglycoside kinases from diverse MDR strains. Journal of Cellular Biochemistry, 2018, 119, 2679-2695.	2.6	21

#	Article	IF	CITATIONS
127	Computational Approaches to Understand Cleavage Mechanism of Amyloid Beta (AÎ ²) Peptide. Neuromethods, 2018, , 263-282.	0.3	3
128	Empirical Scoring Functions for Structure-Based Virtual Screening: Applications, Critical Aspects, and Challenges. Frontiers in Pharmacology, 2018, 9, 1089.	3.5	185
129	In-Silico Prediction and Modeling of the Quorum Sensing LuxS Protein and Inhibition of AI-2 Biosynthesis in Aeromonas hydrophila. Molecules, 2018, 23, 2627.	3.8	18
130	Repurposing Thioridazine (TDZ) as an anti-inflammatory agent. Scientific Reports, 2018, 8, 12471.	3.3	22
131	Prediction of enzymatic pathways by integrative pathway mapping. ELife, 2018, 7, .	6.0	30
132	Designing Algorithms To Aid Discovery by Chemical Robots. ACS Central Science, 2018, 4, 793-804.	11.3	64
133	Bioinformatics approaches for new drug discovery: a review. Biotechnology and Genetic Engineering Reviews, 2018, 34, 243-260.	6.2	40
134	Application of Virtual Screening Approaches for the Identification of Small Molecule Inhibitors of the Methyllysine Reader Protein Spindlin1. Methods in Molecular Biology, 2018, 1824, 347-370.	0.9	5
135	Thiopurine Drugs Repositioned as Tyrosinase Inhibitors. International Journal of Molecular Sciences, 2018, 19, 77.	4.1	12
136	Scavenging of superoxide by a membrane-bound superoxide oxidase. Nature Chemical Biology, 2018, 14, 788-793.	8.0	71
137	Mechanism of imipenem resistance in metalloâ€Î²â€lactamases expressing pathogenic bacterial spp. and identification of potential inhibitors: An in silico approach. Journal of Cellular Biochemistry, 2019, 120, 584-591.	2.6	4
138	Structure-Based Virtual Screening of High-Affinity ATP-Competitive Inhibitors Against Human Lemur Tyrosine Kinase-3 (LMTK3) Domain: A Novel Therapeutic Target for Breast Cancer. Interdisciplinary Sciences, Computational Life Sciences, 2019, 11, 527-541.	3.6	10
139	Peptide Similarity Search Based and Virtual Screening Based Strategies to Identify Small Molecules to Inhibit CarD–RNAP Interaction in M. tuberculosis. International Journal of Peptide Research and Therapeutics, 2019, 25, 697-709.	1.9	11
140	Mechanism of Action of VP1-001 in cryAB(R120G)-Associated and Age-Related Cataracts. , 2019, 60, 3320.		25
141	Essentials of Bioinformatics, Volume II. , 2019, , .		1
142	DockNmine, a Web Portal to Assemble and Analyse Virtual and Experimental Interaction Data. International Journal of Molecular Sciences, 2019, 20, 5062.	4.1	6
143	Broken mirror symmetry, incommensurate spin correlations, and B2g nematic order in iron pnictides. Physical Review B, 2019, 100, .	3.2	15
144	Identification of flavonoids as regulators of YbeY activity in Liberibacter asiaticus. Environmental Microbiology, 2019, 21, 4822-4835.	3.8	6

#	Article	IF	CITATIONS
145	InPrNa: A Tool for Insight Into Protein–Nucleic Acids Interaction Information. IEEE Access, 2019, 7, 140375-140382.	4.2	3
146	Heteroaryl Phosphonates as Noncovalent Inhibitors of Both Serine- and Metallocarbapenemases. Journal of Medicinal Chemistry, 2019, 62, 8480-8496.	6.4	28
147	Molecular Docking: Shifting Paradigms in Drug Discovery. International Journal of Molecular Sciences, 2019, 20, 4331.	4.1	890
148	A Free Web-Based Protocol to Assist Structure-Based Virtual Screening Experiments. International Journal of Molecular Sciences, 2019, 20, 4648.	4.1	16
149	Repurposed Molecules: A New Hope in Tackling Neglected Infectious Diseases. , 2019, , 119-160.		9
150	Molecular Docking: A Structure-Based Approach for Drug Repurposing. , 2019, , 161-189.		22
151	ImmtorLig_DB: repertoire of virtually screened small molecules against immune receptors to bolster host immunity. Scientific Reports, 2019, 9, 3092.	3.3	2
152	Cloud-Based High Throughput Virtual Screening in Novel Drug Discovery. Lecture Notes in Computer Science, 2019, , 250-278.	1.3	12
153	3,17β-Bis-sulfamoyloxy-2-methoxyestra-1,3,5(10)-triene and Nonsteroidal Sulfamate Derivatives Inhibit Carbonic Anhydrase IX: Structure–Activity Optimization for Isoform Selectivity. Journal of Medicinal Chemistry, 2019, 62, 2202-2212.	6.4	14
154	Structure-Based Stepwise Screening of PPARÎ ³ Antagonists as Potential Competitors with NCOA1 Coactivator Peptide for PPARÎ ³ CIS Site. International Journal of Peptide Research and Therapeutics, 2019, 25, 1369-1377.	1.9	7
155	Rational discovery of novel type-III FTF antagonists to competitively suppress TIF-2 coactivation in liver cancer. Journal of Receptor and Signal Transduction Research, 2019, 39, 304-311.	2.5	2
156	Medicinal chemistry: an effect of a desolvation penalty of an amide group in the development of kinase inhibitors. Chemical Papers, 2019, 73, 71-84.	2.2	3
157	Advances and challenges in drug design against tuberculosis: application of in silico approaches. Expert Opinion on Drug Discovery, 2019, 14, 35-46.	5.0	10
158	FtsA as a cidal target for <i>Staphylococcus aureus</i> : Molecular docking and dynamics studies. Journal of Cellular Biochemistry, 2019, 120, 7751-7758.	2.6	31
159	In silico analysis of plasmodium falciparum CDPK5 protein through molecular modeling, docking and dynamics. Journal of Theoretical Biology, 2019, 461, 254-267.	1.7	14
160	Research update and opportunity of non-hormonal male contraception: Histone demethylase KDM5B-based targeting. Pharmacological Research, 2019, 141, 1-20.	7.1	12
161	Advances in distributed computing with modern drug discovery. Expert Opinion on Drug Discovery, 2019, 14, 9-22.	5.0	12
162	Structure-based selection of human metabolite binding P4 pocket of DRB1*15:01 and DRB1*15:03, with implications for multiple sclerosis. Genes and Immunity, 2019, 20, 46-55.	4.1	8

		CITATION REPORT	
#	Article	IF	CITATIONS
163	A small molecule chaperone rescues the stability and activity of a cancerâ€associated variant of NAD(P)H:quinone oxidoreductase 1 <i>inÂvitro</i> . FEBS Letters, 2020, 594, 424-438.	2.8	7
164	Docking Finds GPCR Ligands in Dark Chemical Matter. Journal of Medicinal Chemistry, 2020, 63, 613-620.	6.4	13
165	In-Silico Identified New Natural Sortase A Inhibitors Disrupt S. aureus Biofilm Formation. International Journal of Molecular Sciences, 2020, 21, 8601.	4.1	29
166	Molecular modeling approach to identify inhibitors of Rv2004c (rough morphology and virulent) Tj ETQq1 1 0.7 tuberculosis. Journal of Biomolecular Structure and Dynamics, 2020, , 1-16.	784314 rgB 3.5	T /Overlock 1 1
167	Interaction of N-succinyl diaminopimelate desuccinylase with orphenadrine and disulfiram. Journal of Molecular Structure, 2020, 1222, 128928.	3.6	7
168	Interaction of N-succinyl-diaminopimelate desuccinylase with flavonoids. Biochimie, 2020, 177, 198-212.	2.6	5
169	Rational molecular targeting of the inter-subunit interaction between human cardiac troponin hcTnC and hcTnl using switch peptide-competitive biogenic medicines. Computational Biology and Chemistry, 2020, 87, 107272.	2.3	1
170	Virtual screening web servers: designing chemical probes and drug candidates in the cyberspace. Briefings in Bioinformatics, 2021, 22, 1790-1818.	6.5	81
171	Novel substituted N-benzyl(oxotriazinoindole) inhibitors of aldose reductase exploiting ALR2 unoccupied interactive pocket. Bioorganic and Medicinal Chemistry, 2021, 29, 115885.	3.0	5
172	Synthesis and evaluation of tiaprofenic acid-derived UCHL5 deubiquitinase inhibitors. Bioorganic and Medicinal Chemistry, 2021, 30, 115931.	3.0	2
173	Peptidomimetics in Silico. Molecular Informatics, 2021, 40, e2000087.	2.5	5
174	Property-Unmatched Decoys in Docking Benchmarks. Journal of Chemical Information and Modeling, 2021, 61, 699-714.	5.4	48
175	Online Resource and Tools for the Development of Drugs Against Novel Coronavirus. Methods in Pharmacology and Toxicology, 2021, , 735-759.	0.2	7
176	Screening of potential anti-HIV compounds from Achyranthes aspera extracts for SARS-CoV-2: An insight from molecular docking study. Journal of Physics: Conference Series, 2021, 1797, 012042.	0.4	6
177	Identification of Potential HCV Inhibitors Based on the Interaction of Epigallocatechin-3-Gallate with Viral Envelope Proteins. Molecules, 2021, 26, 1257.	3.8	9
179	Molecular docking identification for the efficacy of some zinc complexes with chloroquine and hydroxychloroquine against main protease of COVID-19. Journal of Molecular Structure, 2021, 1231, 129979.	3.6	41
180	OcimumÂbasilicumÂ(kemangi)Âintervention on powder and microencapsulatedÂSpirulina platensisÂand itsÂbioactiveÂmolecules. F1000Research, 0, 10, 485.	1.6	0
181	Structure-Based Design of First-Generation Small Molecule Inhibitors Targeting the Catalytic Pockets of AID, APOBEC3A, and APOBEC3B. ACS Pharmacology and Translational Science, 2021, 4, 1390-1407.	4.9	11

#	Article	IF	CITATIONS
182	Virtual screening of potential anticancer drugs based on microbial products. Seminars in Cancer Biology, 2022, 86, 1207-1217.	9.6	6
183	Main protease inhibitors and drug surface hotspots for the treatment of COVID-19: A drug repurposing and molecular docking approach. Biomedicine and Pharmacotherapy, 2021, 140, 111742.	5.6	15
184	The extracellular region of bovine milk butyrophilin exhibits closer structural similarity to human myelin oligodendrocyte glycoprotein than to immunological BTN family receptors. Biological Chemistry, 2021, 402, 1187-1202.	2.5	4
185	Structure-based drug designing strategy to inhibit protein-protein-interactions using in silico tools. , 2021, , 139-171.		0
188	Docking with SwissDock. Methods in Molecular Biology, 2019, 2053, 189-202.	0.9	55
189	Informing Mechanistic Toxicology with Computational Molecular Models. Methods in Molecular Biology, 2012, 929, 139-165.	0.9	7
190	Probing Riboswitch Binding Sites with Molecular Docking, Focused Libraries, and In-line Probing Assays. Methods in Molecular Biology, 2014, 1103, 141-151.	0.9	5
191	Identification of a Small Molecule Inhibitor of RAD52 by Structure-Based Selection. PLoS ONE, 2016, 11, e0147230.	2.5	55
192	Identification of a Potential Inhibitor Targeting MurC Ligase of the Drug Resistant Pseudomonas aeruginosa Strain through Structure-Based Virtual Screening Approach and In Vitro Assay. Current Pharmaceutical Biotechnology, 2019, 20, 1203-1212.	1.6	3
193	Drug Repositioning Through Network Pharmacology. Current Topics in Medicinal Chemistry, 2016, 16, 3646-3656.	2.1	57
194	The Comparison of Docking Search Algorithms and Scoring Functions. Advances in Medical Technologies and Clinical Practice Book Series, 2016, , 99-127.	0.3	8
195	Molecular Docking Technique to Understand Enzyme-Ligand Interactions. , 2017, , 727-746.		1
196	Molecular screening and docking analysis of LMTK3 and AKT1 combined inhibitors. Bioinformation, 2018, 14, 499-503.	0.5	9
197	Systems Biology Study of Yeast Mitogen Activated Protein Kinase (MAPK) Cascade for Novel Drug Target Identification against Fungal Pathogens. International Journal of Bioscience, Biochemistry, Bioinformatics (IJBBB), 2013, , 149-153.	0.2	Ο
198	Structural and Computational Approaches in Drug Design for G Protein-Coupled Receptors. , 2015, , 479-489.		2
199	Molecular Docking at a Glance. Advances in Medical Technologies and Clinical Practice Book Series, 2016, , 1-38.	0.3	1
200	Molecular Docking Technique to Understand Enzyme-Ligand Interactions. Advances in Medical Technologies and Clinical Practice Book Series, 2016, , 246-266.	0.3	0
201	Online Molecular Docking Resources. Advances in Medical Technologies and Clinical Practice Book Series, 2016, , 360-379.	0.3	0

# 202	ARTICLE Online Molecular Docking Resources. , 2017, , 941-959.	IF	CITATIONS
203	The Comparison of Docking Search Algorithms and Scoring Functions. , 2017, , 820-849.		0
204	Molecular Docking at a Glance. , 2017, , 764-803.		0
205	Using 3D Structural Information in Computational Design. , 2017, , 101-119.		0
206	Neuropharmacology in Flux: Molecular Modeling Tools for Understanding Protein Conformational Shifts in Alzheimer's Disease and Related Disorders. Neuromethods, 2018, , 573-611.	0.3	1
207	Combinatorial Designing of Novel Lead Molecules Towards the Putative Drug Targets of Extreme Drug-Resistant Mycobacterium tuberculosis: A Future Insight for Molecular Medicine. , 2019, , 233-281.		0
209	OcimumÂbasilicumÂ(kemangi)Âintervention on powder and microencapsulatedÂSpirulina platensisÂand itsÂbioactiveÂmolecules. F1000Research, 2021, 10, 485.	1.6	2
210	Ultrahigh Throughput Protein–Ligand Docking with Deep Learning. Methods in Molecular Biology, 2022, 2390, 301-319.	0.9	3
211	Molecular docking-based computational platform for high-throughput virtual screening. CCF Transactions on High Performance Computing, 2022, 4, 63-74.	1.7	23
212	Hydroxamic Acid as a Potent Metal-Binding Group for Inhibiting Tyrosinase. Antioxidants, 2022, 11, 280.	5.1	7
213	Computational Chemistry and Molecular Modelling Basics. Chemical Biology, 2017, , 1-38.	0.2	9
214	New Inhibitors of Laccase and Tyrosinase by Examination of Cross-Inhibition between Copper-Containing Enzymes. International Journal of Molecular Sciences, 2021, 22, 13661.	4.1	3
215	Discovery of Kinase and Carbonic Anhydrase Dual Inhibitors by Machine Learning Classification and Experiments. Pharmaceuticals, 2022, 15, 236.	3.8	0
216	OcimumÂbasilicumÂ(kemangi)Âintervention on powder and microencapsulatedÂSpirulina platensisÂand itsÂbioactiveÂmolecules. F1000Research, 0, 10, 485.	1.6	0
217	Drugsniffer: An Open Source Workflow for Virtually Screening Billions of Molecules for Binding Affinity to Protein Targets. Frontiers in Pharmacology, 2022, 13, 874746.	3.5	7
218	History and Present Scenario of Computers in Pharmaceutical Research and Development. , 2022, , 1-38.		1
220	Protein-Based Virtual Screening Tools Applied for RNA–Ligand Docking Identify New Binders of the preQ ₁ -Riboswitch. Journal of Chemical Information and Modeling, 2022, 62, 4134-4148.	5.4	10
221	Structure-Based Discovery of Negative Allosteric Modulators of the Metabotropic Glutamate Receptor 5. ACS Chemical Biology, 2022, 17, 2744-2752.	3.4	5

#	Article	IF	CITATIONS
222	DrugRep: an automatic virtual screening server for drug repurposing. Acta Pharmacologica Sinica, 2023, 44, 888-896.	6.1	21
223	Systematic Investigation of Docking Failures in Large-Scale Structure-Based Virtual Screening. ACS Omega, 2022, 7, 39417-39428.	3.5	6
224	Antitumor activity of a pexidartinib bioisostere inhibiting CSF1 production and CSF1R kinase activity in human hepatocellular carcinoma. Chemico-Biological Interactions, 2023, 369, 110255.	4.0	3
225	Perceiver CPI: a nested cross-attention network for compound–protein interaction prediction. Bioinformatics, 2023, 39, .	4.1	11
226	Pesticide informatics expands the opportunity for structure-based molecular design and optimization. , 2022, 1, 139-147.		11
227	Docking strategies. , 2023, , 243-258.		2
228	Hic Sunt Dracones: Molecular Docking in Uncharted Territories with Structures from AlphaFold2 and RoseTTAfold. Journal of Chemical Information and Modeling, 2023, 63, 2218-2225.	5.4	6
229	In silico screening of potential compounds from begonia genus as 3CL protease (3Cl pro) SARS-CoV-2 inhibitors. Journal of Public Health in Africa, 0, , .	0.4	0
230	Principles of computational drug designing and drug repurposing—An algorithmic approach. , 2023, , 129-146.		0
231	A deep learning model for drug screening and evaluation in bladder cancer organoids. Frontiers in Oncology, 0, 13, .	2.8	1
232	Naphtho[2,1-b]furan derived triazole-pyrimidines as highly potential InhA and Cytochrome c peroxidase inhibitors: Synthesis, DFT calculations, drug-likeness profile, molecular docking and dynamic studies. Journal of Molecular Structure, 2023, 1287, 135685.	3.6	9
233	Exploration of Indolo[3,2c]isoquinoline derived triazoles as potential antimicrobial and DNA cleavage agents: Synthesis, DFT calculations, and molecular modeling studies. Bioorganic Chemistry, 2023, 137, 106598.	4.1	6
234	Structure-based discovery of novel cruzain inhibitors with distinct trypanocidal activity profiles. European Journal of Medicinal Chemistry, 2023, 257, 115498.	5.5	5
235	Establishing mammalian GLUT kinetics and lipid composition influences in a reconstituted-liposome system. Nature Communications, 2023, 14, .	12.8	4
236	Catalytic inhibitor of Protein Phosphatase 5 activates the extrinsic apoptotic pathway by disrupting complex II in kidney cancer. Cell Chemical Biology, 2023, 30, 1223-1234.e12.	5.2	1
237	Discovery of potent STAT3 inhibitors using structure-based virtual screening, molecular dynamic simulation, and biological evaluation. Frontiers in Oncology, 0, 13, .	2.8	0
239	Redocking the PDB. Journal of Chemical Information and Modeling, 0, , .	5.4	1
240	MulinforCPI: enhancing precision of compound–protein interaction prediction through novel perspectives on multi-level information integration. Briefings in Bioinformatics, 2023, 25, .	6.5	0

#	Article	IF	CITATIONS
241	Docking for Molecules That Bind in a Symmetric Stack with SymDOCK. Journal of Chemical Information and Modeling, 2024, 64, 425-434.	5.4	0
242	DockOpt: A Tool for Automatic Optimization of Docking Models. Journal of Chemical Information and Modeling, 2024, 64, 1004-1016.	5.4	0
243	Inhibitory effects of menthol, B12N12, B16N16, Al12N12, Al16N16, and their complexes on tumor necrosis factor-alpha (TNF-α) and their potential anti-inflammatory activity: A study using DFT and molecular docking. Inorganic Chemistry Communication, 2024, 162, 112187.	3.9	0
244	TECHNIQUES AND ALGORITHMS FOR STRUCTURE-BASED VIRTUAL SCREENING (SBVS): AN OVERVIEW. Indian Drugs, 2024, 61, 7-17.	0.1	0
245	The eugenol functionalized B12N12 and B16N16 cages as potential inhibitors of TNF- $\hat{l}\pm$ and HER2 receptors. Polyhedron, 2024, 254, 116935.	2.2	0